Diethylmalonic acid, 1-bromo-3,3,3-trifluoroprop-2-yl dodecyl ester

Inchi: InChI=1S/C22H38BrF3O4/c1-4-7-8-9-10-11-12-13-14-15-16-29-19(27)21(5-2,6-3)20(28)

InchiKey: PZSUKTMAIWOWOP-UHFFFAOYSA-N

Formula: C22H38BrF3O4

SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)OC(CBr)C(F)(F)F

Mol. weight [g/mol]: 503.43

Physical Properties

Property code	Value	Unit	Source
gf	-900.35	kJ/mol	Joback Method
hf	-1571.79	kJ/mol	Joback Method
hfus	54.48	kJ/mol	Joback Method
hvap	83.88	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	7.126		Crippen Method
mcvol	358.530	ml/mol	McGowan Method
pc	942.10	kPa	Joback Method
rinpol	2341.00		NIST Webbook
rinpol	2341.00		NIST Webbook
tb	912.41	K	Joback Method
tc	1117.19	K	Joback Method
tf	533.43	K	Joback Method
vc	1.403	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1161.78	J/mol×K	912.41	Joback Method
cpg	1178.76	J/mol×K	946.54	Joback Method
cpg	1194.61	J/mol×K	980.67	Joback Method
cpg	1209.42	J/mol×K	1014.80	Joback Method
cpg	1223.27	J/mol×K	1048.93	Joback Method
cpg	1236.22	J/mol×K	1083.06	Joback Method
cpg	1248.35	J/mol×K	1117.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume